

The 4D-Var assimilation of ozone-sensitive infrared radiances measured by IASI

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An analysis of ozone that is constrained only by observations of ultraviolet backscatter has an obvious limitation. These data are not available at night-time. A system has been developed to exploit ozone information from infrared radiances measured by IASI which suffer no such sampling problems related to the position of the sun. It has been found that, relative to a baseline system that has no ozone observations, the use of IASI significantly improves the fit to independent ozone estimates from the Aura MLS. Indeed this improvement is, in some areas, comparable to or better than that obtained when more established ozone estimates from UV sensors are assimilated. One area where the assimilation of IASI is found to be clearly beneficial is in the winter high latitudes and southern polar night. Copyright © 2010 Royal Meteorological Society

Key Words: IR radiances; ozone; 4DVAR; NWP

Received 19 May 2010; Revised 20 August 2010; Accepted 8 September 2010; Published online in Wiley Online Library

Citation: Han W, McNally AP. 2010. The 4D-Var assimilation of ozone-sensitive infrared radiances measured by IASI. *Q. J. R. Meteorol. Soc.* **136**: 2025–2037. DOI:10.1002/qj.708

1. Introduction

A number of operational global numerical weather prediction (NWP) systems currently have an analysis of ozone that is constrained by observations of ultraviolet (UV) backscatter from instruments such as Solar Backscatter Ultraviolet Radiometer (SBUV). However, an obvious limitation of these data is that they are not available at night-time. We thus have half of the globe unobserved daily and an entire polar region unobserved for much of the winter season. Data from the Microwave Limb Sounder (MLS) on board the Aura satellite have no such sampling problems and have been identified as a valuable source of high-quality ozone information. However, from the viewpoint of an operational NWP centre, there is a problem in that there is no envisaged operational follow-on to this instrument. There is also no heritage of similar data provided by previous instruments that could be used to support climate and reanalysis studies. While data from the MLS will be exploited by operational centres during the periods when they are available, it is unwise to develop an operational reliance upon the information provided by such observations. These considerations lead to a strong incentive to be able to extract

ozone information from infrared (IR) sources. With these, there are no sampling problems related to the position of the sun, a guaranteed operational provision of future data and an extensive historical record to study climate.

Another potentially important benefit from the successful extraction of ozone information from IR radiances is the possibility of constraining the stratospheric wind analysis via advection tracing. It has been demonstrated that a 4D-Var assimilation system can derive useful tropospheric wind information from humidity-sensitive radiances by advecting humidity features to improve the analysis fit to observations (Peubey and McNally, 2009). IR sensors (with ozone channels) are carried on multiple polar-orbiting platforms which together provide a frequent temporal sampling at higher latitudes. At lower latitudes, IR sensors on geostationary platforms provide very high temporal resolution. If ozone feature tracing (Peuch *et al.*, 2000) can successfully be extracted from IR ozone data, the resulting wind information could be even more significant due to the absence of any other sources of wind data in the stratosphere.

Ozone-sensitive IR radiance observations have been available for many years from the High-resolution InfraRed Sounder (HIRS), Meteosat Visible and InfraRed

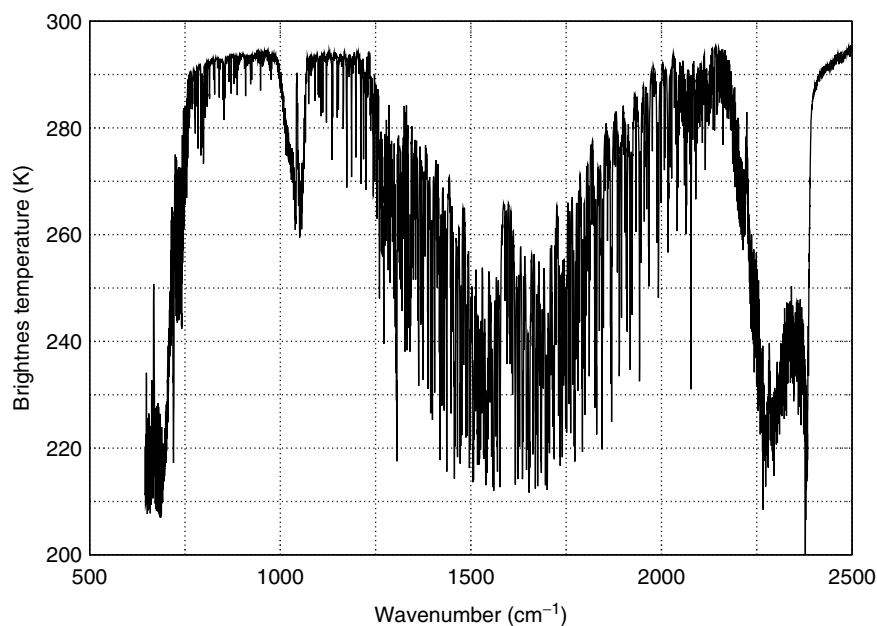


Figure 1. The IASI IR spectrum showing the ozone band at approximately 1000 wavenumbers ($9\ \mu\text{m}$) computed from a standard midlatitude profile.

Imager (MVIRI), Geostationary Operational Environmental Satellite (GOES) and Spinning Enhanced Visible and InfraRed Imager (SEVIRI) instruments. However, it is probably fair to say that these have been conspicuously underused in global NWP compared to the use of UV backscatter data. There are a number of reasons for this. Firstly, the ozone information comes from IR channels that have a significant sensitivity to clouds and surface emission. Thus errors in the detection of cloud contamination and the characterization for surface emissivity and skin temperature can potentially undermine the useful ozone signal in the data. Secondly, the observed radiances and the radiative transfer (RT) model used in the interpretation of the observations are both prone to biases. This problem is of course not unique to ozone-sensitive data and applies to all radiance observations. However, there is significantly less unbiased independent ozone information available for the diagnosis and correction of systematic errors in ozone-sensitive radiances compared to that available to detect and correct biases in temperature-sensitive radiances.

In recent years, radiance observations from advanced IR sounders such as the Atmospheric Infrared Sounder (AIRS) and Infrared Atmospheric Sounding Instrument (IASI) have become available and the significant impact of temperature and humidity information from these on NWP has been well documented (McNally *et al.*, 2006; Collard and McNally, 2009). Much of this impact undoubtedly comes from the very high information content of these data by virtue of the fine-resolution spectral sampling of the IR spectrum. However, there are two other important characteristics that enhance the utility of data from these instruments. Firstly, the availability of many hundreds of channels with a gradually increasing sensitivity to clouds has led to the development of advanced cloud-detection techniques (McNally and Watts, 2003). These not only have a more stringent capability to detect cloud contamination, but also allow the use of some radiance data above low-level cloud cover. Secondly, the spectral and radiometric calibration of the advanced sounders has been demonstrated

to be very accurate and stable. Similar advances in RT models (Matricardi *et al.*, 2004) and spectroscopy (in some part assisted by the availability of these data for validation) now results in systematic errors over large parts of the measured spectrum being extremely small.

It is thus now timely to investigate to what extent these helpful characteristics of advanced IR sounders can allow a more successful exploitation of ozone information from AIRS and IASI than has been possible previously with low-spectral-resolution IR data.

This paper deals with the extraction of ozone information from IASI and begins with a brief overview of the ozone information content and the ECMWF ozone analysis. Results from three different assimilation systems are shown. A baseline with no direct ozone observations, a system using ozone estimates from UV observations and a system using ozone-sensitive IR radiances from IASI. The differences between the resulting ozone analyses are discussed in terms of improving (or otherwise) the fit to independent ozone estimates from MLS and ozone sondes. The paper concludes with a summary and a look forward to future developments.

2. The IASI radiance data and their information content

The part of the IASI spectrum with greatest sensitivity to ozone is the region around $9\ \mu\text{m}$. Here there is an absorption band centre (strongest attenuation) located at $9.6\ \mu\text{m}$ and symmetric weaker absorption either side, blending into the long-wave window part of the spectrum (Figure 1). It can be seen that, even at its maximum, the absorption due to ozone is weaker than that due to water vapour around $6\ \mu\text{m}$ and significantly weaker than the attenuating effects of carbon dioxide at 15 and $4\ \mu\text{m}$. Consequently, while the IASI channels around $9\ \mu\text{m}$ provide information on ozone, they retain a significant sensitivity to the surface emission (in clear-sky conditions) and indeed clouds when they are present.

Jacobians for two IASI ozone channels, 1585 (strong absorption) and 1671 (weak absorption) are shown in Figure 2 for a typical midlatitude atmosphere (Jacobians

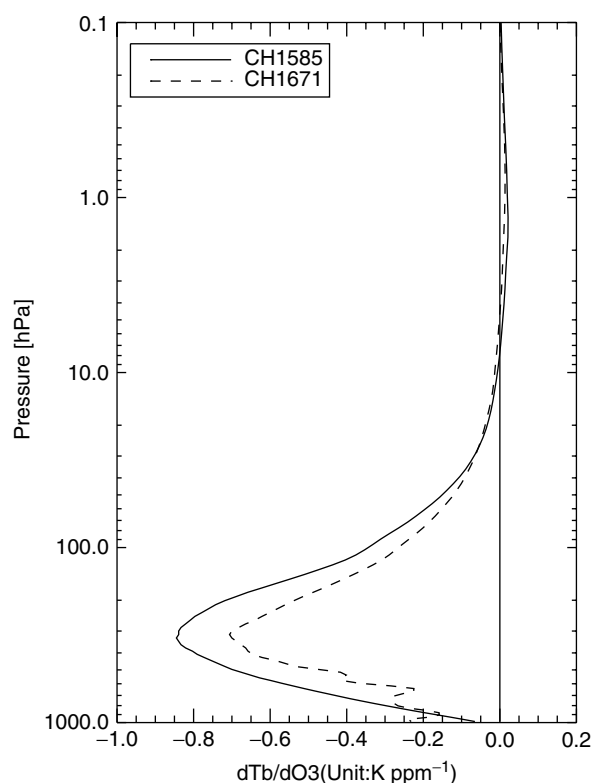


Figure 2. IASI midlatitude ozone Jacobians for channels 1585 and 1579. The quantity shown is the change in brightness temperature (K) for a unit change of ozone mass mixing ratio (mg kg^{-1}), as a function of pressure level.

in the Tropics are rather similar). It is important to note that the perturbation used in forming the Jacobians is a unit change in ozone mass mixing ratio. This choice of variable results in the peak sensitivity being located in the upper troposphere and lower stratosphere. If the perturbation were a percentage change in ozone, the Jacobian would peak much higher in the atmosphere, near the altitude of maximum ozone concentration (typically 20 hPa). Ozone mass mixing ratio has been chosen in this context as this is the variable currently used in the 4D-Var analysis system.

The similarity between the strong absorbing channel (1585) and the weak absorbing channel (1671) suggests that the IASI data do not convey a significant amount of information on the vertical distribution of ozone. Thus the assimilation of IASI ozone radiances will rely on prior background constraints (i.e. the short-range forecast of ozone and its error covariance) to control the vertical distribution of ozone information. Background errors for ozone mass mixing ratio in the current ECMWF 4D-Var system are shown in Figure 3. The errors are largest near the level of maximum ozone concentration. The geographic variation of the error is only slight and inter-level correlations are rather local.

We expect the IASI radiances to have largest impact on the analysis at a level where the convolution of the background-error profile with the Jacobians is a maximum (note this convolution is only an illustrative proxy for what happens inside a data assimilation scheme). This is shown in Figure 4 and indicates that the impact should be in the lower stratosphere and some way below the level of maximum ozone concentration.

3. Cloud screening and bias correction of IASI ozone channels

Radiances from IASI have been used operationally at ECMWF since June 2007 closely following the system developed for the assimilation of AIRS data. However, until now the focus has been on exploiting temperature and humidity information from these advanced IR sounders and ozone channels have not been used. Data from advanced IR sounders are screened for clouds using the algorithm described in McNally and Watts (2003), where clear channels in a potentially cloud-affected scene are identified. The algorithm examines departures of the observed radiances from clear-sky computed values (from the model background) and searches for the characteristic signature of cloud. In the long-wave temperature sounding band of IASI, we have confidence that anomalous signatures in the radiance departures are due to cloud as the temperature information provided by the NWP model background is rather accurate. However, in the IASI ozone band larger errors in the background ozone information could potentially be misinterpreted as cloud contamination. This would result in data that could have been assimilated to improve the ozone analysis being rejected before they can be used. To guard against this, independent cloud information diagnosed from the long-wave temperature sounding band is interrogated to infer which channels in the ozone band can be used in a particular scene.

Systematic errors in satellite radiance observations are removed by the Variational Bias Correction scheme (VarBC; Auligné *et al.*, 2007). The underlying assumption is that the background state provided by the NWP system is reasonably unbiased (primarily by virtue of its assimilation of high-quality radiosonde data). Any large-scale mean signal in the radiance departures is considered a bias in the satellite observations (or the associated radiative transfer model) and is automatically removed each analysis cycle. For temperature sounding channels, the assumption of an unbiased state being provided by the NWP system is reasonably valid, but again a reduced confidence in the quality of the ozone background information has led to a modified approach for ozone channels. For this study we have chosen to anchor the VarBC system by fixing the bias correction for one of the most ozone-sensitive IASI channels (1585 located at $9.61 \mu\text{m}$) to a constant value. This ensures that the ozone radiance observations are not wrongly corrected to the potentially biased ozone information coming from the NWP system. Only one channel is fixed to allow the VarBC to establish corrections that remove inter-channel biases between ozone channels. (Corrections for these other channels are parametrized with a global offset and three scan-angle-dependent predictors, although in practice the scan-dependent biases are very small.) Obviously this approach places a great emphasis on the value at which the anchor channel bias correction is fixed. Figure 5 shows the mean observed minus background radiance departure in channel 1585 from a baseline system that assimilates no ozone data. In this context negative departures –where the background calculated radiances are warmer than the observations –indicate that the background is deficient in ozone concentration (positive radiance departures indicate the opposite). Equivalent mean departure statistics for independent ozone estimates obtained from MLS are shown in Figure 6. The MLS data are averaged over three

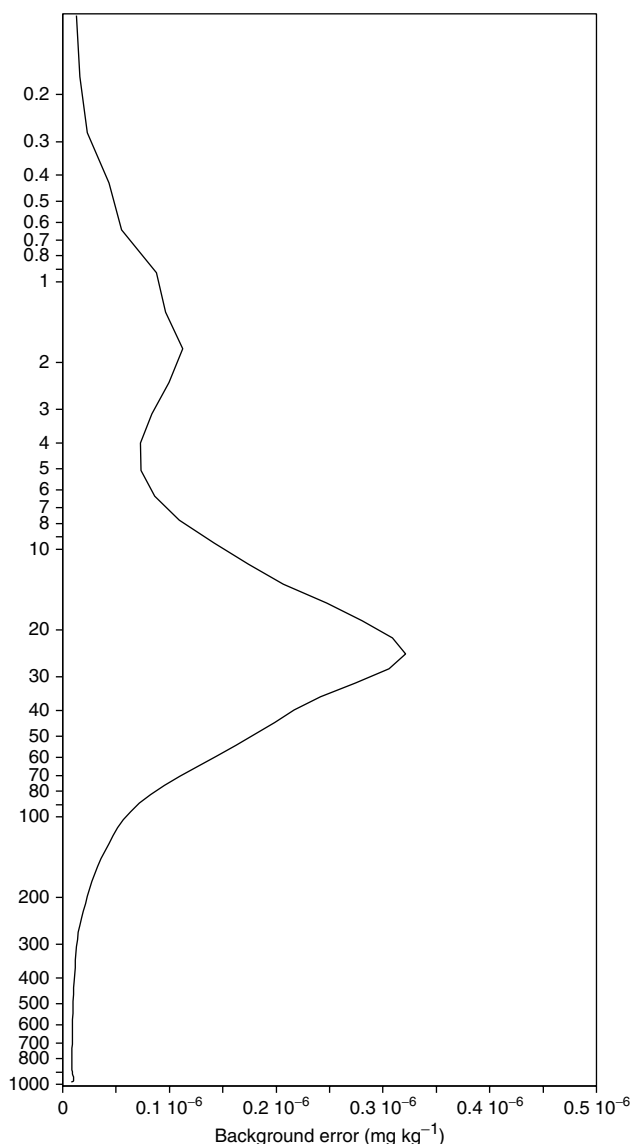


Figure 3. Globally averaged standard deviation of background errors for ozone mass mixing ratio (mg kg^{-1}) for the summer period (15 to 30 June 2009), as a function of pressure level.

levels between 30 and 50 hPa in an attempt to be more representative of the ozone at levels to which IASI radiances are most sensitive. In this context, positive departures indicate that the MLS has more ozone than the background. Qualitatively the patterns from IASI channel 1585 and the MLS appear rather similar with both observations suggesting that the dominant mean signal is an ozone deficiency in the southern midlatitudes, switching to a slight excess of ozone over the South Pole. In the Tropics and at high northern latitudes, there is also an excess of ozone. This degree of agreement between the MLS and the IASI radiance data has led to the decision to fix the bias correction for the anchor channel 1585 at zero. While it is likely that there are other sources of bias in this IASI channel (e.g. due to residual cloud contamination and radiative transfer errors), this choice is likely to be better than anchoring to the mean radiance departure from the NWP background which is clearly biased. The resulting bias corrections used in other channels (after two weeks of evolution in VarBC) are shown in Figure 7.

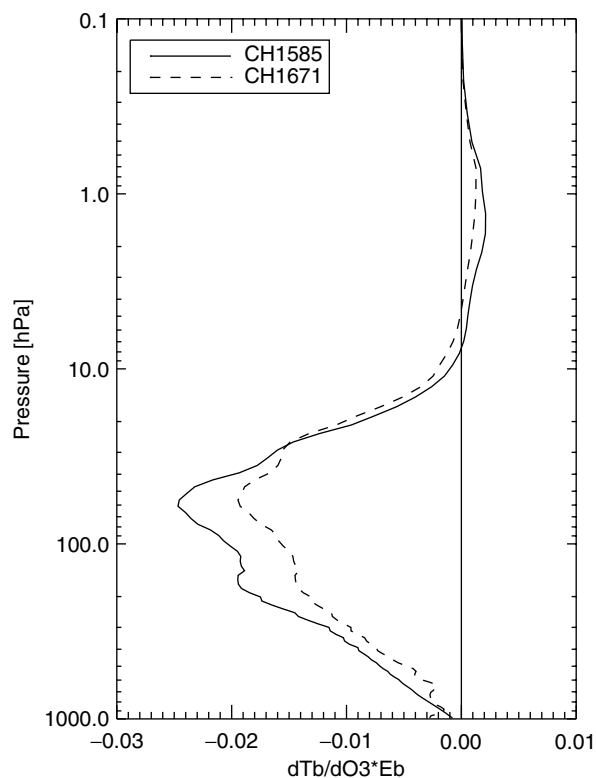


Figure 4. Ozone background errors convolved with Jacobians.

4. Ozone assimilation experiments with UV data and IASI radiances

Ozone analysis in the ECMWF 4D-Var system is described in Dethof and Hólm (2004), and currently assimilates ozone products derived from observations of UV backscatter made by the SBUV (Bhartia *et al.*, 1996) (presented to the analysis in six layers, the lowermost 16 hPa to the surface) and the Aura Ozone Monitoring Instrument (OMI) (presented to the analysis as total column only). Some important recent modifications to the analysis should be noted. Firstly, the forecast model component of the observation operator that links wind adjustments to changes in ozone concentration has been artificially cut (Dee *et al.*, 2009). This step was taken to suppress large erroneous wind and temperature increments found in the stratospheric analyses that were associated with the tracing of biases between the ozone observations and model background. Secondly, the VarBC scheme, initially developed for radiance data, has been extended to the correction of ozone observations. In the current operational configuration, the SBUV is used as an anchor (with zero bias correction applied) and the OMI data corrected adaptively within the analysis (Dragani, 2009).

For the purposes of this study, we construct three different assimilation systems. Firstly, a baseline that uses all conventional and satellite observations currently assimilated by ECMWF, but with all ozone data removed. This is run down for two weeks prior to the start of the study period to lose memory of the initial ozone conditions and reach equilibrium (in terms of error saturation). Secondly, a system identical to the baseline except that ozone estimates from SBUV and OMI are used (essentially the current operational configuration). Finally, a system is run that is identical to the baseline, but additionally assimilates 16 IASI radiances from the $9\mu\text{m}$ (approximately 1000

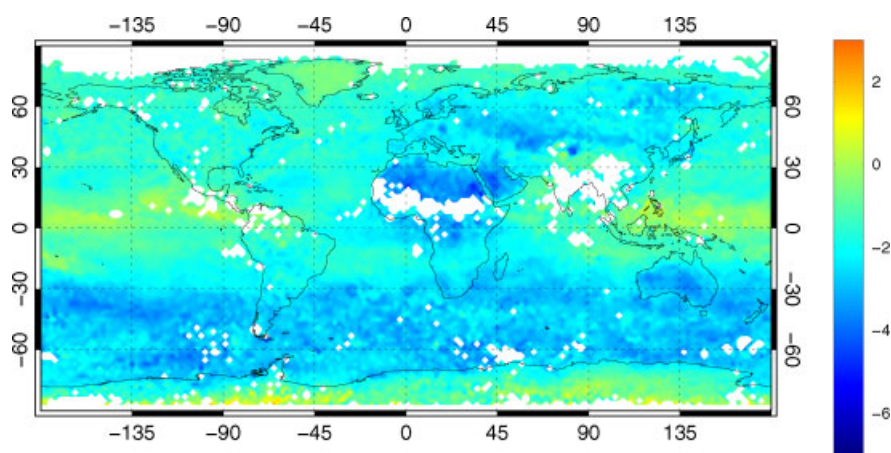


Figure 5. Mean observed-minus-background radiance departures (K) from the baseline in channel 1585 during the summer period (15 to 30 June 2009). This figure is available in colour online at wileyonlinelibrary.com/journal/qj

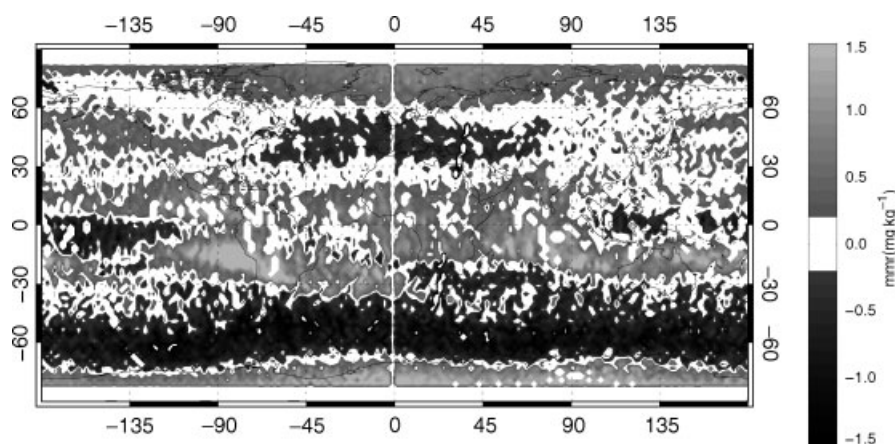


Figure 6. Mean baseline-analysis minus MLS ozone mass mixing ratio departures (mg kg^{-1}) for the summer period (15 to 30 June 2009). The MLS data is averaged over three levels between 30 and 50 hPa, to be consistent with the levels to which IASI radiances are most sensitive.

wavenumbers) ozone band. Note that the IASI data are added on top of the baseline rather than the operational UV configuration. This choice allows us to understand the ozone changes due to IASI more clearly without the complicating factor of interactions with other ozone observations. It also allows us to gauge the usefulness of the IASI ozone information by comparing to analyses based on the more established UV ozone observations. All assimilation experiments have been run using version CY35R3 of the ECMWF forecasting and assimilation system at horizontal resolution T511 (approximately 40 km grid) with 91 levels in the vertical.

Two separate periods have been tested: 1 May 2009 to 31 July 2009, capturing the Northern Hemisphere (NH) summer, and the opposite season 1 January 2009 to 29 February 2009. Examples of the data coverage in the two systems are shown in Figure 8. It can be seen that the use of UV data is limited by the availability of sunlight, leaving the winter pole unobserved. The use of IASI observations is more uniform, although data are lost when clouds are present. In the first configuration tested here, data over land and sea ice are excluded. This is a conservative step and follows the operational usage of temperature and humidity channels from IASI. It is known that a poor knowledge of the surface emission (either the surface emissivity or skin temperature) over land can limit the skill and reliability of the cloud detection scheme. In addition, errors in the surface

emission can potentially alias into erroneous adjustments of ozone if these signals are misinterpreted by the assimilation system. Later in this study, we present results where IASI ozone data are used over land and compare with the analyses when these data are excluded.

5. Changes to the ozone analysis and comparison with MLS

In this section we compare the changes due to the assimilation of IASI radiances with those from UV data and to what extent these changes influence the fit of the resulting ozone analyses to ozone estimates from the MLS (note that changes in polar night are treated separately). MLS on the Aura satellite provides near-global estimates of ozone in the stratosphere and upper troposphere (82°S to 82°N). The effective vertical resolution of the MLS data is estimated to be around 3 or 4 km in the upper troposphere and stratosphere (Froidevaux *et al.*, 2006), and the horizontal resolution typically estimated to be around 200 km. The accuracy of the most recent version (2.2) of the MLS data is well documented (Livesey *et al.*, 2008) and suggests errors better than 10% in the in the upper troposphere and better than 5% in the stratosphere. While the MLS data cannot be regarded as a validation *truth*, they are arguably the most accurate globally available product. Studies that have investigated the impact of assimilating

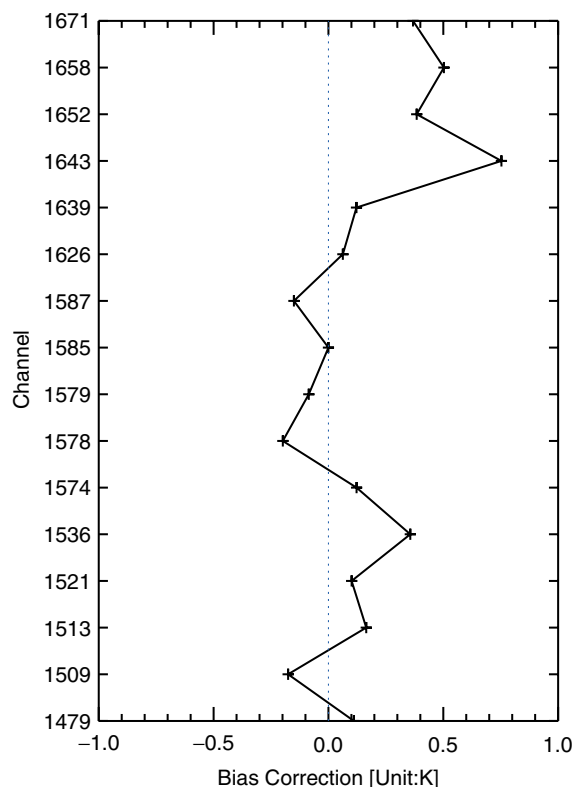


Figure 7. Bias corrections (K) estimated by VarBC for IASI ozone channels when channel 1585 is anchored at zero. This figure is available in colour online at wileyonlinelibrary.com/journal/qj

MLS data have generally drawn rather positive conclusions as to their value (Jackson, 2007; Feng *et al.*, 2008).

5.1. The Northern Hemisphere winter period

In the NH midlatitudes, the comparison of the baseline with MLS in Figure 9 indicates a systematic overestimation of ozone centred around 20 hPa (near the level of maximum ozone concentration) and an underestimation (of similar magnitude) above and below. The use of IASI radiances causes an increase of ozone centred on 200 hPa (Figure 10) that produces an analysis that is completely unbiased with respect to the MLS in the troposphere. The use of IASI also causes a removal of ozone above (again improving the fit to MLS), but this removal appears too strong around 50 hPa. The UV data add ozone around 200 hPa (improving the agreement with MLS), but the dominant signal above is an addition around 30 hPa that degrades the MLS fit.

In the Tropics, the MLS suggests that the baseline has a fairly deep layer with systematic underestimation of ozone. The assimilation of IASI increases the ozone concentration to improve the fit to MLS. The UV data also add ozone, but this appears excessive and slightly misplaced in the vertical, only marginally improving the agreement with MLS.

In the Southern Hemisphere (SH) midlatitudes the baseline system displays an extremely strong systematic overestimation of ozone at 10 hPa and an equally strong underestimation only a few levels below at 30 hPa, extending down below 100 hPa. Apart from a slight improvement below 100 hPa, the IASI data are clearly unable to resolve such a feature and fail to improve the fit to MLS higher in the atmosphere. In contrast, the assimilation of UV data causes

changes that improve the agreement with MLS, particularly at higher southern latitudes.

5.2. The Northern Hemisphere summer period

In the NH midlatitudes, the comparison of the baseline with MLS in Figure 11 again indicates a systematic overestimation of ozone centred around 20 hPa (stronger than observed during the winter season) and a very slight underestimation below. The use of IASI radiances produces only modest changes (Figure 10), but these do improve mean agreement with MLS. Again the UV data do a good job of reducing the overestimation of ozone at higher latitudes, but the removal is excessive and extends to lower levels where the fit to MLS is degraded.

In the Tropics the MLS suggests that the baseline has an ozone error similar in magnitude, but opposite in sign (i.e. overestimation) to that seen in the winter period. However, the error is significantly narrower in vertical extent than observed for the winter and switches to a weak underestimation of ozone below. The IASI radiances are sensitive to the underestimation and correct accordingly at lower levels, but cause an addition of ozone that extends to the levels above –degrading the fit to MLS. Conversely the UV data are sensitive to, and attempt to correct, the overestimation above, but the removal extends too far down and degrades the fit to MLS below. In the SH midlatitudes, the baseline system again displays an extremely strong systematic overestimation of ozone around 20 hPa and a strong underestimation only a few levels below. As was the case in the winter period, the IASI data are unable to resolve this strong dipole feature, but do cause a useful addition of ozone in the lower levels to improve the MLS fit. The UV data do a good job of removing the excess ozone in the upper levels, although the addition of ozone in the lower levels is slightly excessive.

5.3. The polar night

As stated in the introduction, one of the main drivers to use IR data is the need to observe ozone in the polar winter when an absence of solar radiation renders UV-based observing systems blind. We now study in more detail the changes to the ozone analysis due to the assimilation of IASI in polar night conditions. Analysis differences compared to the baseline system are shown in Figure 12 averaged over the NH summer period for the Antarctic region (where of course it is winter). Two levels are shown, roughly corresponding to 15 hPa and 50 hPa. At the upper level (15 hPa) it is striking that, despite there being no UV ozone observations at high southern latitudes (as it is dark), the assimilation of ozone data at lower latitudes leads to a large removal of ozone at the pole. In addition to the normal horizontal spreading of increments by the analysis system, the UV data can force changes far beyond their local influence by affecting the large-scale thermodynamic transport of ozone. The removal of ozone in the midlatitudes as far as 50°S (where there are observations) seems reasonable, but the removal of ozone that extends further south into the polar night is excessive according to the MLS estimates. At the same level (15 hPa) the assimilation of IASI causes a much weaker removal of ozone, only marginally improving the fit to MLS. However, there is no spreading of the changes to the South Pole. At the lower level (50 hPa) there is an addition of ozone

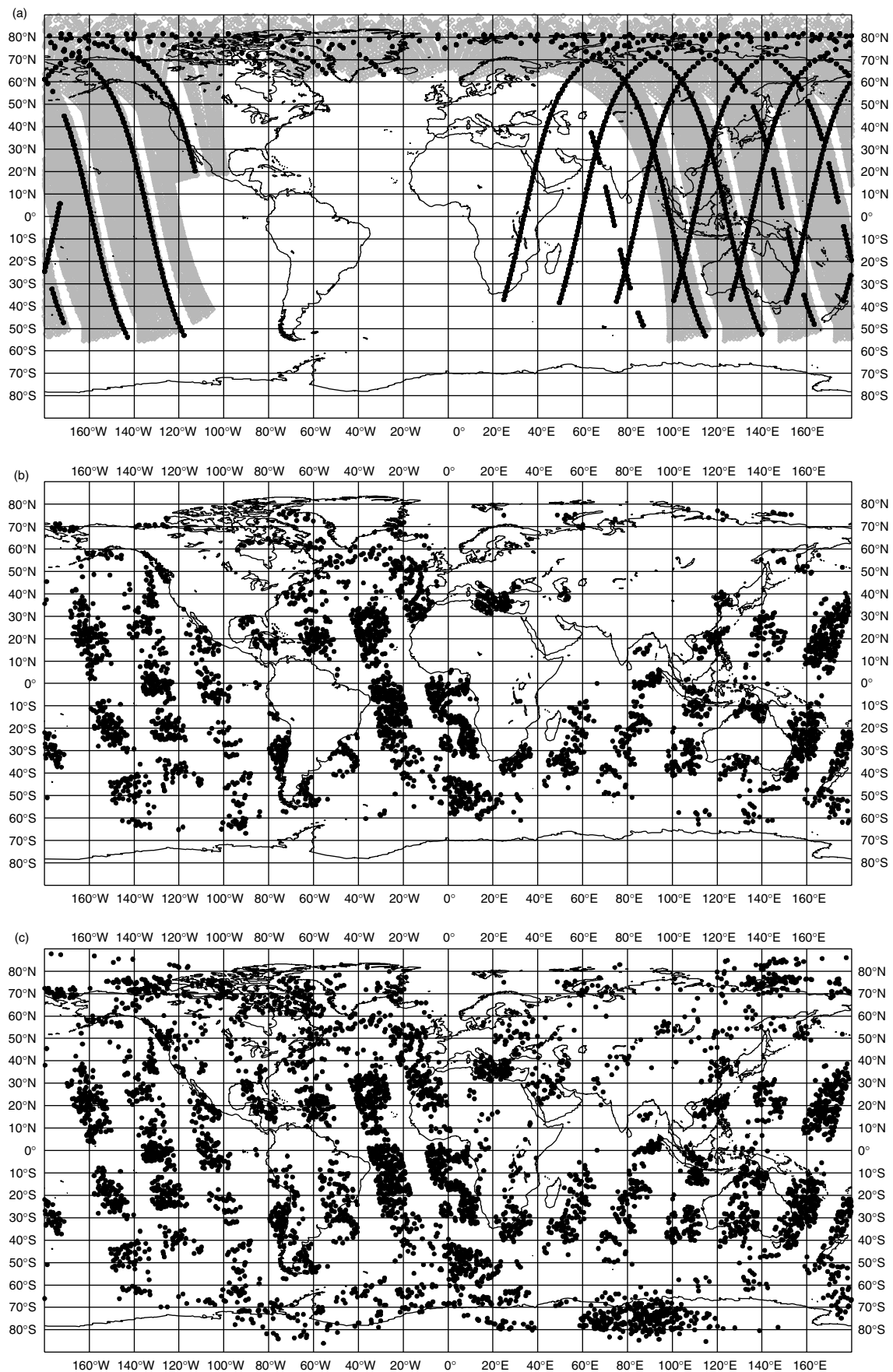


Figure 8. Data coverage of (a) UV data from SBUV (black) and OMI (grey), (b) IASI data over ocean and (c) IASI data including land and sea ice from a typical 12-hour period in the summer experiment.

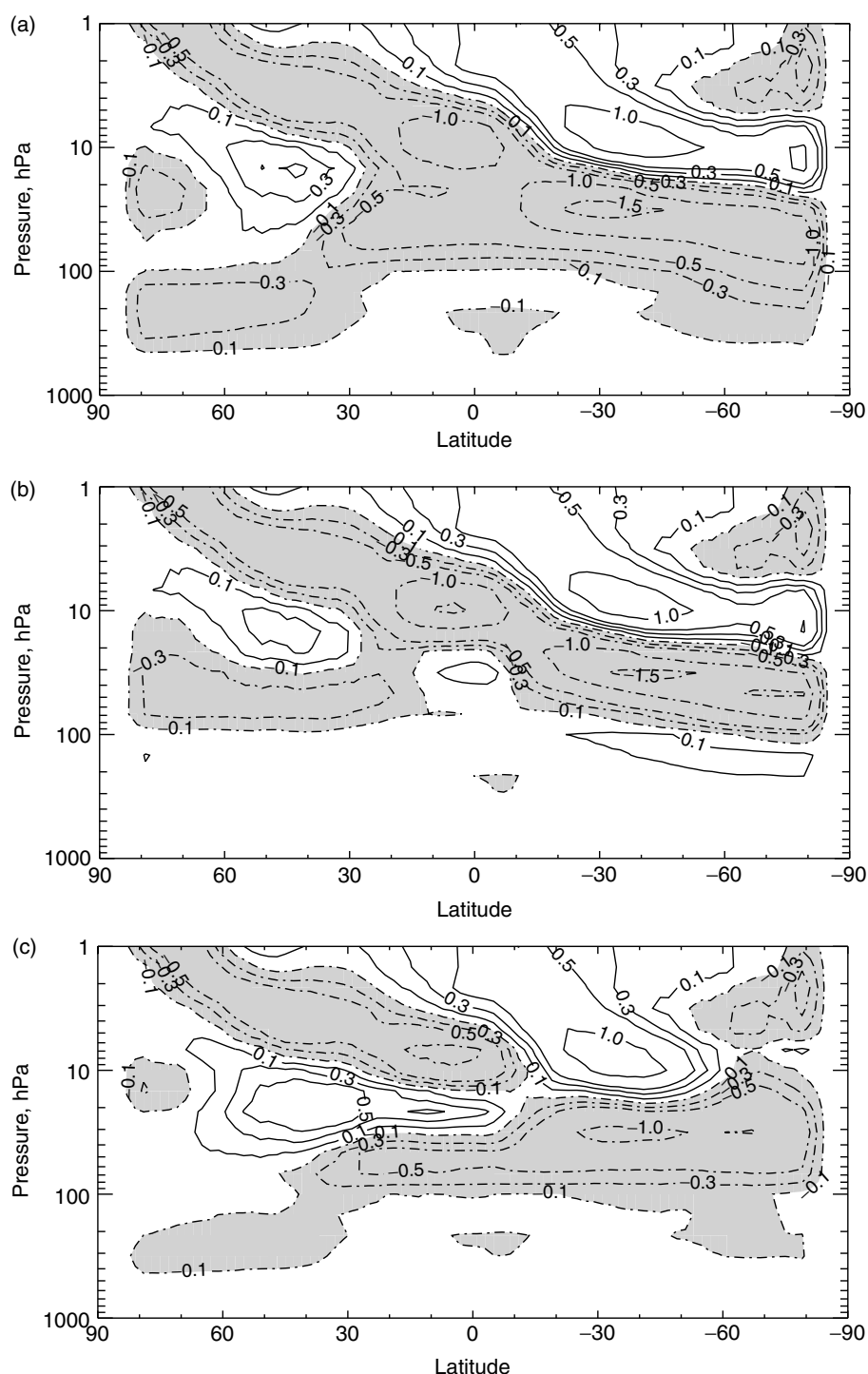


Figure 9. Zonally averaged mean differences (over the winter period) of the analyzed ozone mass mixing ratio (mg kg^{-1}) minus MLS ozone, for (a) the baseline, (b) the IASI system and (c) the UV system. The shaded contours indicate that the analysis has less ozone than the MLS, open contours indicate the opposite.

due to the UV data which again spreads and strengthens all the way to the South Pole. The addition of ozone at lower latitudes (where there are UV observations) improves the fit to MLS, but again the extension of this addition southwards is opposite to the changes suggested by MLS. The MLS indicates that the underestimation of ozone in the baseline at low latitudes switches to an overestimation at the South Pole. The assimilation of IASI radiances also adds ozone at low latitudes, but crucially correctly captures the change in sign further south where ozone is then removed and improves the fit to MLS.

6. Changes to the ozone analysis and comparison with ozone sondes

Ozone estimates from radiosonde data are obtained from the World Ozone and Ultraviolet Radiation Data Centre (WOUDC; <http://www.woudc.org>), and the Southern Hemisphere Additional Ozonesondes (SHADOZ) network. There are a variety of sensor technologies used, but the most common are Electrochemical Concentration Cells (ECC). For these the errors are typically estimated around 10–15% in the troposphere, improving to better than 5% through

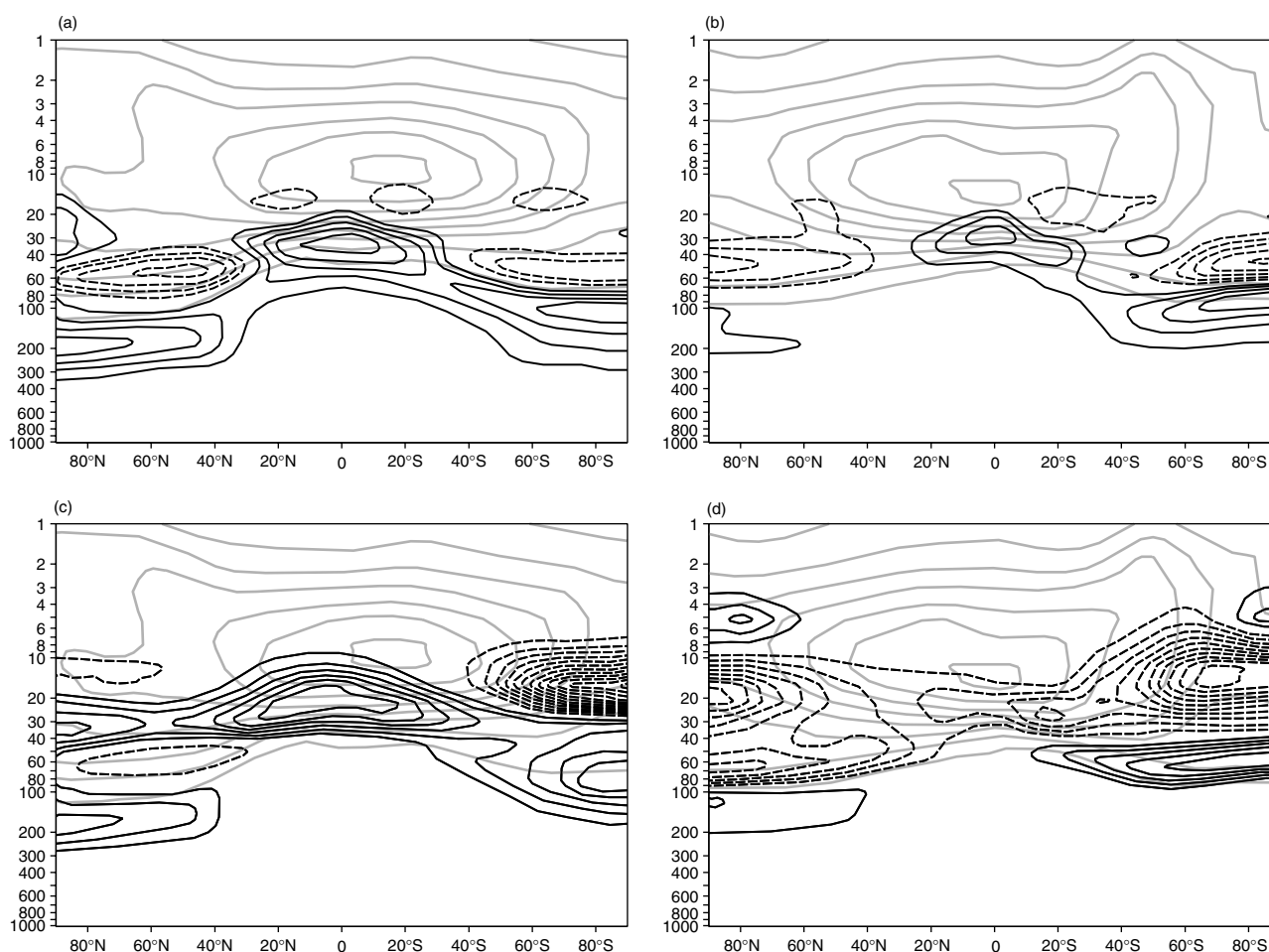


Figure 10. Zonally averaged mean analysis difference (as a function of pressure level) of the IASI analyzed ozone mass mixing ratio (mg kg^{-1}) minus the baseline: (a) for winter and (b) for summer. (c, d) is as (a, b), but for UV analyzed ozone. Contours are at intervals of 0.1, solid indicating positive changes, dashed indicating negative changes. The grey contours show the mean ozone analysis of the baseline system in each case.

much of the stratosphere. (Komhyr *et al.*, 1995). While ozone sonde data provide arguably the most accurate independent measurements of ozone in the atmosphere, they suffer from a very poor temporal and spatial coverage of the globe. Most are in the NH, but even here the sampling is such that very different results are obtained site to site when compared with analyses (and the spread at individual sites is large due to the small sample sizes). For this reason we have decided to group the data into large area averages (NH and SH). The results are generally consistent with the findings when the analysis changes are compared with MLS data. An example is shown in Figure 13 for the NH summer season (averaged over the same period as the MLS comparison of figure). We see a more dramatic indication than shown by the MLS that the baseline analysis overestimates the peak ozone concentration. The assimilation of IASI removes some excess ozone, but not nearly enough according to the sonde data. Similarly the addition of ozone by IASI below 100 hPa (that clearly improved the fit to MLS) does not significantly improve the fit to the sonde data.

7. Use of IASI radiance data over land

The IASI ozone channels have a significant sensitivity to emission from the surface and errors in the modelling of surface temperature and surface emissivity can potentially alias into erroneous adjustments of ozone. In addition, a

poor modelling of the surface emission can reduce the reliability of the cloud detection scheme. This is why the bulk of this investigation has focussed on using IASI data only over ice-free ocean. However, we now compare this cautious approach with an assimilation system where IASI radiances are additionally used over sea ice and land (for the NH summer period only). Over most parts of the globe, the zonal mean analysis changes are found to be rather similar to the analysis when only ocean data are used (and are therefore not shown). There is a very slight strengthening of some signals, indicating that the land/ice-based radiance observations are generally reinforcing the information of the ocean data, and these lead to a correspondingly small change in the mean fit to MLS. A larger impact of land data is seen in the standard deviation of the ozone analysis compared to MLS. This is shown in Figure 14 where the standard deviation of the baseline system has been subtracted so that negative values indicate a decrease (improved fit to MLS compared to the baseline). The additional use of IASI land data reduces the random errors, particularly over the northern midlatitudes and Antarctica, more than the system that uses only IASI over ocean. This indicates that, while the extra data may have only a small effect on the large-scale mean ozone analysis, they do provide an important additional constraint upon random errors.

The area where land data seem to have largest impact is over the southern polar region. It was observed in the

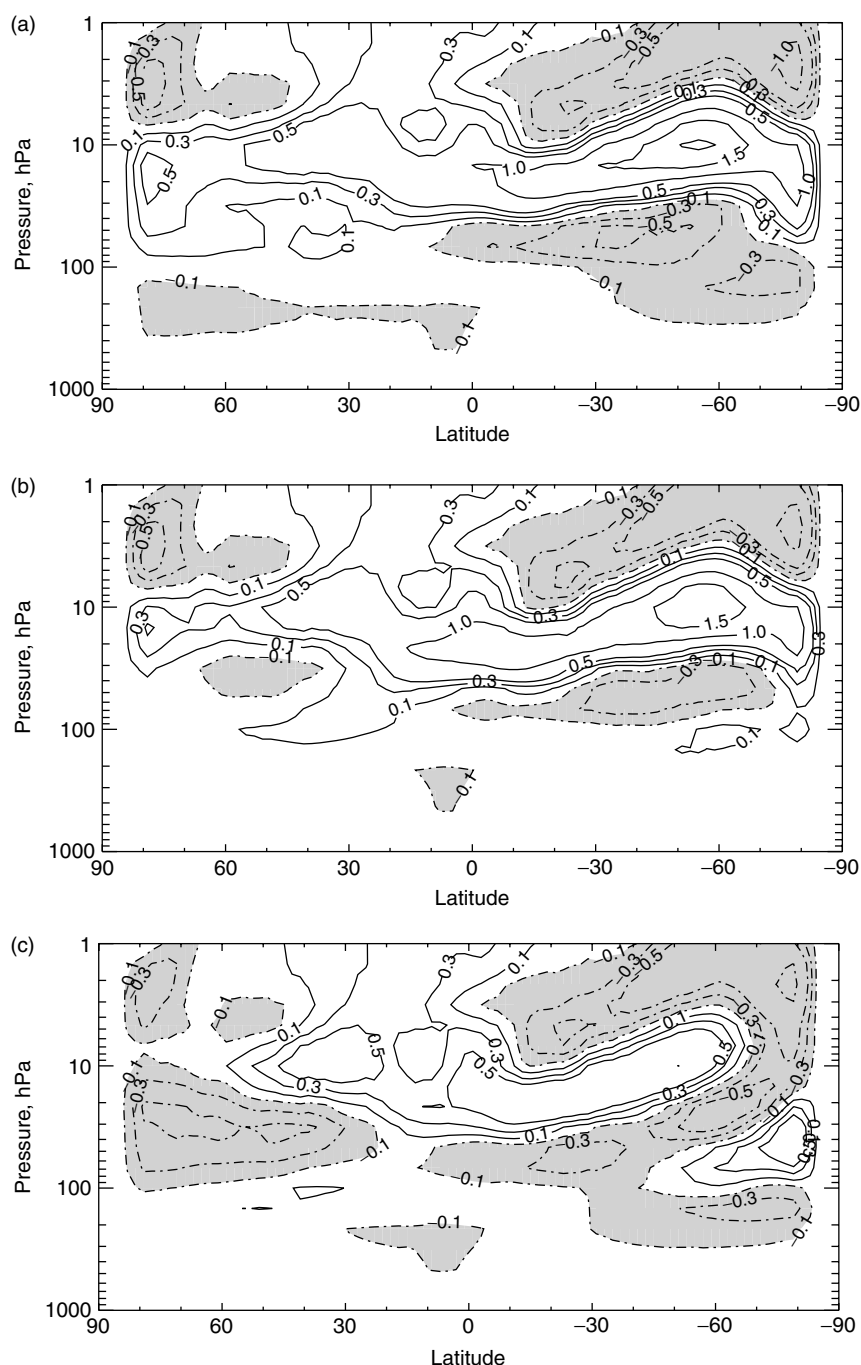


Figure 11. As Figure 9, but for the summer period.

previous section that the assimilation of IASI data was able to capture the reversal of sign (adding ozone in the midlatitudes, but then removing ozone further south at 50 hPa) that the assimilation based on UV data had missed. The additional use of IASI data over the Antarctic land mass significantly strengthens the removal of ozone at this level (figure), clearly improving both the mean and random agreement with MLS ozone estimates south of 70°S.

8. Summary and discussion

This study has investigated the value of assimilating ozone-sensitive IR radiances from IASI. It has been found that, relative to a baseline system that has no ozone observations, the use of IASI significantly improves the fit

to independent ozone estimates from the Aura MLS. Indeed this improvement is, in some areas, comparable or better than that obtained when more established ozone estimates from UV sensors are assimilated.

In broad terms, the impact of assimilating the IASI data is largest in the upper troposphere and lower stratosphere, consistent with the known sensitivity of the radiances as described by the ozone Jacobian. The assimilation of IASI has only a marginal effect at altitudes near the maximum ozone concentration. This is in contrast to, but therefore complementary with, the impact of assimilating UV data which tend to constrain ozone more strongly at higher levels.

One area where the assimilation of IASI is clearly beneficial is in the winter high latitudes and southern polar night. The

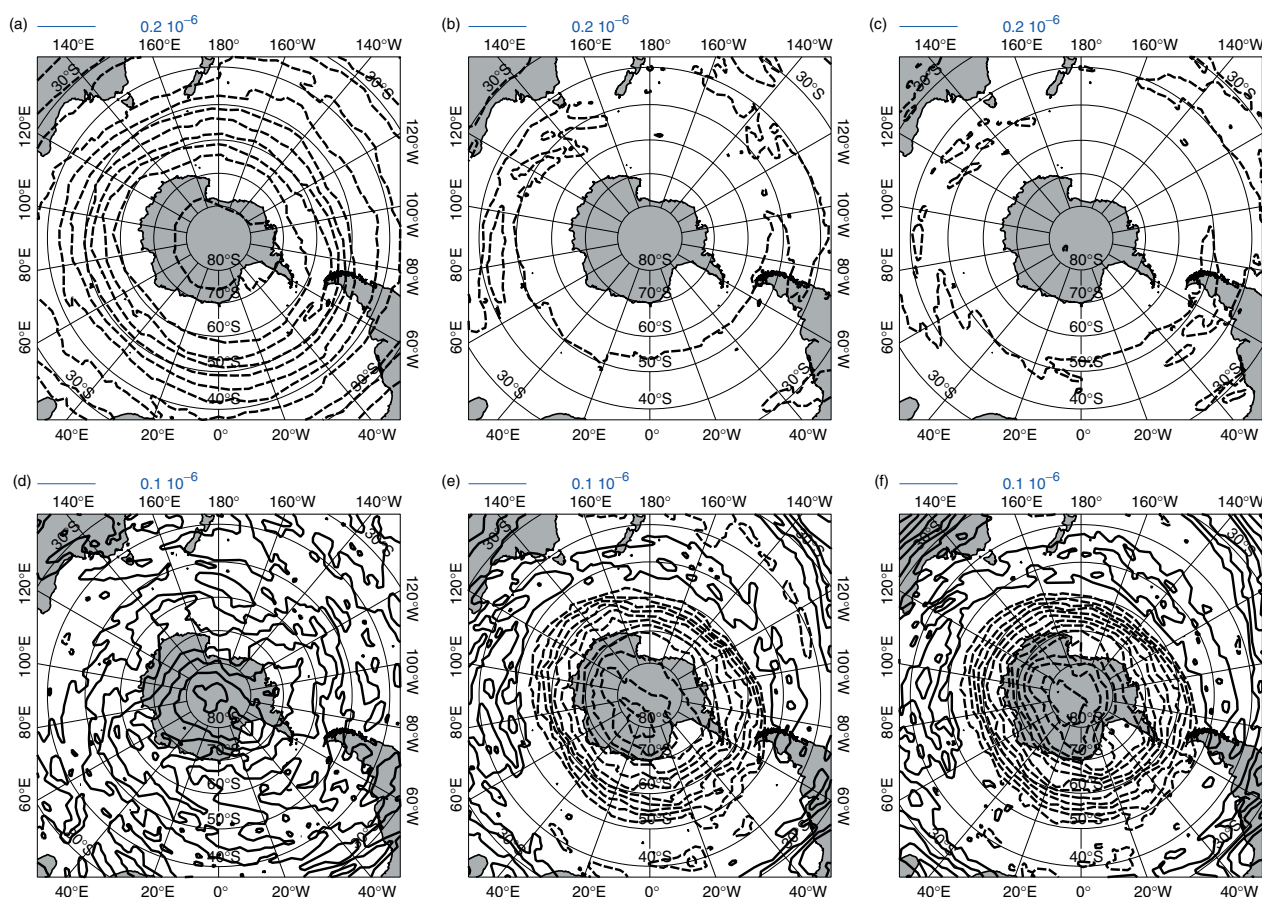


Figure 12. Mean analysis differences for the summer period of the analyzed ozone mass mixing ratio (mg kg^{-1}) minus the baseline at (a, b, c) 15 hPa and (d, e, f) 50 hPa. (a, d) show the UV analyses minus baseline, (b, e) the IASI analyses minus baseline, and (c, f) IASI including land and sea ice minus baseline. Solid contours indicate an increase of ozone, dashed contours a removal of ozone relative to the baseline. This figure is available in colour online at wileyonlinelibrary.com/journal/qj

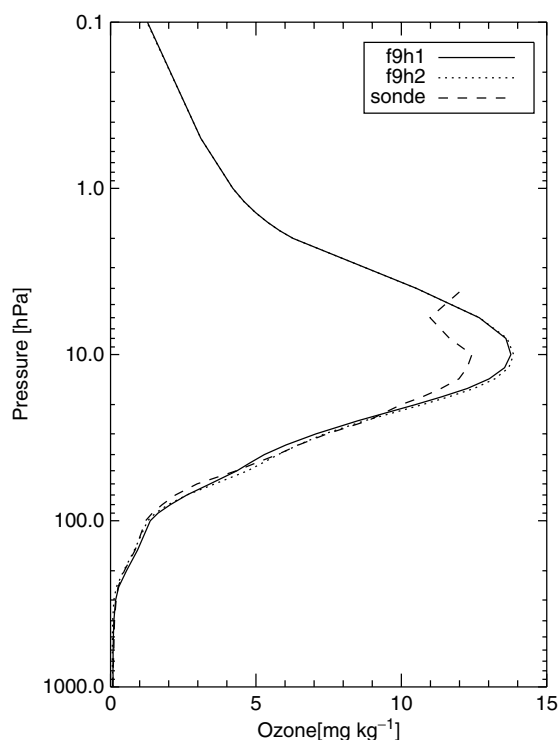


Figure 13. Comparison of the ozone mass mixing ratio (mg kg^{-1}) from the IASI analyses with ozone sonde data from the Northern Hemisphere in the summer period. The solid line is the IASI analysis, the dotted line the baseline and the dashed line the sonde data.

UV-based system was seen to spread erroneous increments into areas where there were no UV ozone data (due to an absence of sunlight). The more homogeneous coverage of IR ozone information did not do this and crucially captured a switch from positive to negative ozone errors that the UV system missed.

While a cautious use of IASI radiances only over sea seems to capture most of the large-scale mean signals over much of the globe, the additional use of IASI data over land appears to have value. The assimilation of land data was found to improve the constraint of random ozone errors in the analysis and produce a better description of ozone in the southern polar night. Despite these encouraging results, concerns remain about the potential detrimental effect that poorly modelled surface emission may have on ozone-sensitive radiances. A much more detailed investigation of different land surfaces in different seasons would be required to gain more confidence in the use of radiances over land.

Results suggest that the current assimilation of a limited number of IASI channels (16) cannot constrain errors with a sharp vertical structure due to the limited vertical resolution of the data. Future studies assimilating a larger proportion of the many hundreds of ozone-sensitive radiances that are measured by IASI may yield marginally better results, but are not expected to significantly improve this weakness.

It should be stressed that the results of these studies are not only indicative of the intrinsic value of the IASI (and indeed UV) ozone data, but equally sensitive to the skill of the

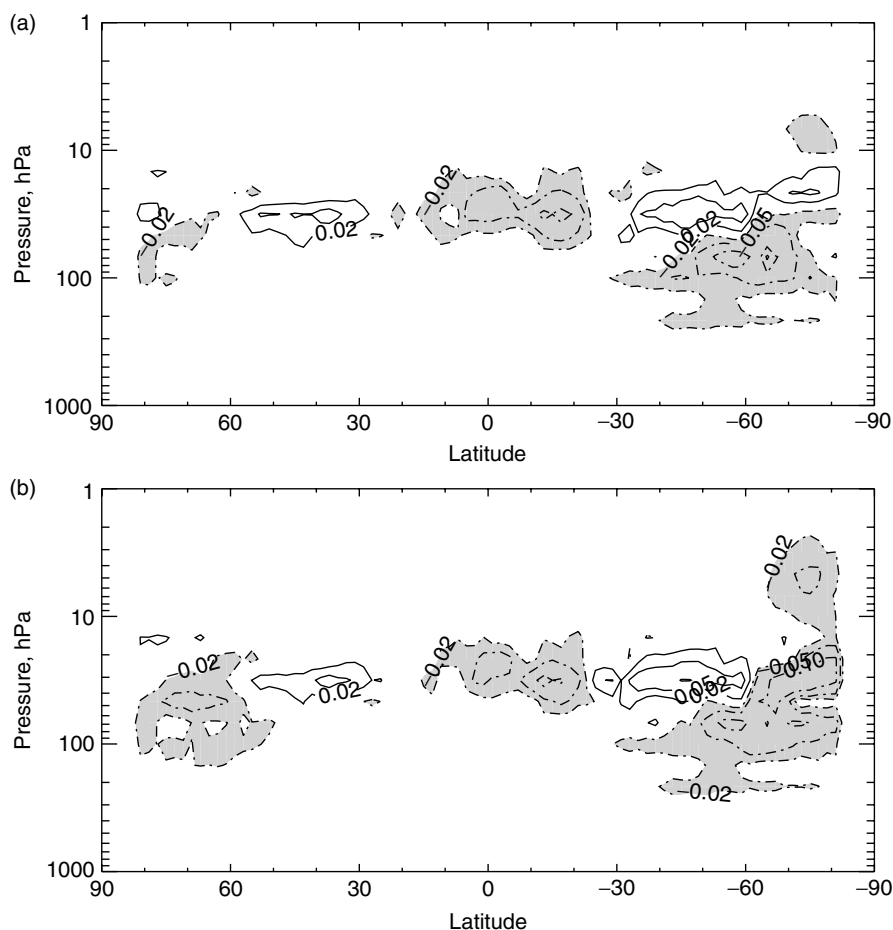


Figure 14. Zonally averaged standard deviation of difference (from the summer period) of the analyzed ozone mass mixing ratio (mg kg^{-1}) minus MLS ozone for (a) the standard IASI system and (b) the IASI system that makes additional use of radiances over land and sea ice. In both cases, the standard deviation of baseline differences has been subtracted so that negative values (shaded contours) indicate the degree of improvement relative to the baseline.

assimilation system. Two areas are of crucial importance. Firstly, the handling of systematic errors in the data has been described here, but there is considerable scope for bias corrections to be optimized. Neither observing system (IASI or UV) consistently improves the fit to MLS data in all areas (which themselves may be biased) and the NWP model is unlikely to be bias-free. The exact choice of bias correction (e.g. a flat global offset or a highly air-mass-dependent correction) and the choice of anchoring will have a fundamental impact on the ozone analysis. Secondly, the IASI data suffer from a lack of vertical resolution and so the role of the assimilation system in distributing information in the vertical is important. (Note that while the UV data are artificially retrieved onto a profile layer grid, the intrinsic vertical resolution of the data is an issue.) This control of increments in the vertical is achieved by the ozone background-error covariance and optimization of this may again have a fundamental impact on the ozone analysis.

It is beyond the scope of this limited study, but an immediate next step is to establish an optimal blend of UV and IR ozone information in the operational analysis exploiting the complementary strengths of both. Similarly the exploitation of ozone information from other IR sounders is a near-term priority. While applying the experience gained with IASI to AIRS should be relatively straightforward, low spectral resolution sounders such as HIRS and SEVIRI are more problematic. Broadband

radiometers are typically more difficult to model (i.e. radiative transfer biases may be larger) and have intrinsically lower vertical resolution. Another important difficulty is that these sensors have fewer ozone-insensitive temperature sounding channels available to assist in the detection of clouds.

An important step for the future is to investigate the potential of ozone-sensitive IR radiances from multiple platforms (in combination with UV data) to constrain errors in the analysis wind field via the 4D-Var tracing. In the current version of the ECMWF 4D-Var, ozone feature tracing is deliberately disabled (in practice by explicitly zeroing any gradient of the ozone data fit with respect to changes in the initial wind field). This pragmatic step was taken as a preventative measure against large erroneous wind and temperature adjustments in the stratosphere associated with the assimilation of biased UV observations under certain conditions. Clearly a precursor to re-activating the tracing mechanism is optimize the current ozone analysis (blending the best information from IR and UV sources along the lines already discussed) and eliminate (as far as possible) any sources of bias.

Another important area that must be investigated in the future is how improvements in the analysis of ozone are preserved in the extended ozone forecasts. This has not been treated in this study due to another pragmatic feature of the current ECMWF system. The radiation scheme of

the forecast model does not use the ozone fields that are forecasted from the initial conditions (i.e. the ozone analysis), but reverts to a climatology estimate of ozone (Morcrette, 2003). It remains to be seen if an improved analysis of ozone coupled with the latest developments in ozone transport and chemistry will allow this crucial link with the radiation scheme to be reinstated.

Acknowledgements

The contribution of Wei Han to this work was funded by the EUMETSAT NWP-SAF Visiting Scientist Program. The authors would like to thank Dr Peter Bauer for his helpful comment on the manuscript and Dr Rossana Dragani for her advice during the study and help in the use of MLS and ozonesonde data.

References

- Auligné T, McNally AP, Dee DP. 2007. Adaptive bias correction for satellite data in a numerical weather prediction system. *Q. J. R. Meteorol. Soc.* **133**: 631–642.
- Bhartia PK, McPeters RD, Mateer CL, Flynn LE, Wellemeyer C. 1996. Algorithm for the estimation of vertical ozone profiles from the backscattered ultraviolet technique. *J. Geophys. Res.* **101**: 18793–18806.
- Collard AD, McNally AP. 2009. The assimilation of Infrared Atmospheric Sounding Interferometer radiances at ECMWF. *Q. J. R. Meteorol. Soc.* **135**: 1044–1058.
- Dee DP. 2003. 'Problems with the assimilation of ozone data'. Tech. Report 739, ECMWF: Reading, UK.
- Dethof A, Hólm EV. 2004. Ozone assimilation in the ERA-40 reanalysis project. *Q. J. R. Meteorol. Soc.* **130**: 2851–2872.
- Dragani R. 2009. 'Monitoring and assimilation of SCIAMACHY, GOMOS and MIPAS retrievals at ECMWF: Technical support for global validation of ENVISAT data products'. Technical Report 21519/08/I-OL. ECMWF: Reading, UK.
- Froidevaux L, Livesey NJ, Read WG, Jiang YB, Jimenez C, Filipiak MJ, Schwartz MJ, Santee ML, Pumphrey HC, Jiang JH, Wu DL, Manney GL, Drouin BJ, Waters JW, Fetzer EJ, Bernath PF, Boone CD, Walker KA, Jucks KW, Toon GC, Margitan JJ, Sen B, Webster CR, Christensen LE, Elkins JW, Atlas E, Lueb RA, Hendershot R. 2006. Early validation analyses of atmospheric profiles from EOS MLS on the Aura satellite. *IEEE Trans. Geosci. Remote Sens.* **44**: 1106–1121.
- Jackson DR. 2007. Assimilation of EOS MLS ozone observations in the Met Office data assimilation system. *Q. J. R. Meteorol. Soc.* **133**: 1771–1788.
- Komhyr WD, Barnes RA, Brothers GB, Lathrop JA, Opperman DP. 1995. Electrochemical concentration cell ozonesonde performance evaluation during STOIC 1989. *J. Geophys. Res.* **100**(D5): 9231–9244.
- Livesey NJ, Filipiak MJ, Froidevaux L, Read WG, Lambert A, Santee ML, Jiang JH, Pumphrey HC, Waters JW, Cofield RE, Cuddy DT, Daffer WH, Drouin BJ, Fuller RA, Jarnot RF, Jiang YB, Knosp BW, Li QB, Perun VS, Schwartz MJ, Snyder WV, Stek PC, Thurstans RP, Wagner PA, Avery M, Browell EV, Cammas JP, Christensen LE, Diskin GS, Gao RS, Jost HJ, Loewenstein M, Lopez JD, Nédélec P, Osterman GB, Sachse GW, Webster CR. 2008. Validation of Aura Microwave Limb Sounder O₃ and CO observations in the upper troposphere and lower stratosphere. *J. Geophys. Res.* **113**: D15S02, DOI: 10.1029/2007JD008805.
- Matricardi M, Chevallier F, Kelly G, Thépaut J-N. 2004. An improved general fast radiative transfer model for the assimilation of radiance observations. *Q. J. R. Meteorol. Soc.* **130**: 153–173.
- McNally AP, Watts PD. 2003. A cloud detection algorithm for high-spectral-resolution infrared sounders. *Q. J. R. Meteorol. Soc.* **129**: 3411–3423.
- McNally AP, Watts PD, Smith JA, Engelen R, Kelly GA, Thépaut J-N, Matricardi M. 2006. The assimilation of AIRS radiance data at ECMWF. *Q. J. R. Meteorol. Soc.* **132**: 935–957.
- Morcrette J-J. 2003. 'Ozone–radiation interactions in the ECMWF forecast system'. Tech. Memo. 375, ECMWF: Reading, UK.
- Peubey C, McNally AP. 2009. Characterization of the impact of geostationary clear-sky radiances on wind analyses in a 4D-Var context. *Q. J. R. Meteorol. Soc.* **135**: 1863–1876.
- Peuch A, Thépaut J-N, Pailleux J. 2000. Dynamical impact of total-ozone observations in a four-dimensional variational assimilation. *Q. J. R. Meteorol. Soc.* **126**: 1641–1659.